

Theory of optical conductivity in detwinned $\text{YBa}_2\text{Cu}_3\text{O}_y$

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We study theoretically the chain and in-plane optical conductivities of detwinned $\text{YBa}_2\text{Cu}_3\text{O}_y$. We elaborate that the chain is superconducting for $y > 6.67$ while insulating for $y < 6.67$ due to the competition between the plane-chain coupling and the antiferromagnetic order, corresponding to a superconductor-insulator transition. Stemming also from the coupling between the plane and chain, a new peak emerges at a low frequency in the in-plane spectra in the superconducting state, while it disappears in the normal state. Our scenario accounts satisfactorily for very recent experiments.

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$\text{YBa}_2\text{Cu}_3\text{O}_y$ (YBCO) is one of the most studied high- T_c superconducting materials. A primary distinction between this system and other cuprates is the presence of the quasi-one-dimensional CuO chain. Though it is widely believed that the main physics in this material is within the CuO_2 plane, the study of electronic properties in the chain and their influence on the superconducting plane may enable us to have a profound understanding on superconductivity in the present system [1, 2, 3, 4]. One of powerful tools to detect the electronic structure is the measurement of optical conductivity. It was reported that a pronounced $a - b$ axis anisotropy exists in the spectra [5, 6, 7, 8, 9, 10, 11], which are strongly enhanced in the chain direction. By subtracting the a -axis spectra from the b -axis (the chain direction) spectra, one can obtain experimentally the spectra contributed by the chain. In this way, the chain electronic structure revealed by the optical experiments shows some unusual features. Several experiments showed that the optical conductivity in the CuO chain exhibits a peak at a finite frequency [5, 6, 7] and approaches to zero in the dc limit, implying that the chain is insulating though the CuO_2 plane is still in the superconducting state. On the other hand, it was also reported that the chain spectra are characterized as a Drude-like peak located at the zero frequency, demonstrating the chain superconductivity [8, 9, 10].

Recently, a detail investigation of the infrared response in the detwinned YBCO [11] provided us a systematic doping dependence of the electrodynamics in the CuO chain. The optical spectra contributed by the chain display a dominant Drude-like peak in the $y = 6.75$ sample. While as y decreases to 6.65, the Drude-like peak will shift to a narrow resonance peak at the finite frequency, indicating that the superconductor-insulator transition occurs in the CuO chain. In fact, the appearance of this transition around $y = 6.65$ may also be inferred from the doping dependence of the superfluid density [10]. A theoretical explanation of the chain superconductivity based on the plane-chain coupling was given by Morr and Balatsky [12], however, an elaboration of the observed

superconductor-insulator phase transition and the insulating nature of the chain is still awaited. In the meantime, another important issue is how the in-plane spectra are influenced by the chain. Very recently, an experiment on detwinned ortho-II phase $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ observed an extra strong peak at 180 cm^{-1} (about 20 meV) in the a -axis optical conductivity in addition to the usually observed Drude-like peak and the mid-infrared (MIR) component in twinned samples [13]. Therefore, a consistent accounting for the optical response in both the plane and chain of the detwinned system is appealing.

In this paper, we demonstrate that the competition of the plane-chain coupling and the antiferromagnetic (AF) order in the chain gives rise to the superconductor-insulator transition in the CuO chain, namely, the proximity superconductivity in the chain is induced by the plane-chain coupling when there is no AF order or it is negligible, while the insulating gap in the optical conductivity is caused by the AF order when its magnitude is appreciable. Starting from a self-consistent mean-field treatment for both the planar and chain Hamiltonian, we extend a simple existing model [14, 15] of the plane-chain coupling to include the emergency of the AF order in the chain at low dopings. Interestingly, we find a step-like rise of the AF order at the oxygen content $y = y_c = 6.67$ which is almost the same as the superconductor-insulator transition point observed experimentally [11]. In the meantime, the chain optical conductivity shows an insulating gap below y_c ; while above y_c , the chain optical conductivity rapidly acquires a Drude-like peak at the dc limit and shows a proximity-induced superconductivity. On the other hand, we find that a new peak occurs at a low frequency ($0.18J \approx 23\text{meV}$ with J as the AF exchange integral) in the in-plane optical conductivity due to the coupling between the plane and chain. These results agree quantitatively with the recent experimental measurements [11, 13], and thus give a consistent picture of the chain and in-plane optical conductivity in the detwinned YBCO.

We start with a Hamiltonian which describes a system

with a plane and a chain per unit cell,

$$H = H_p + H_c + H_I, \quad (1)$$

where H_p describes the CuO₂ plane:

$$\begin{aligned} H_p = & -t_p \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{p\dagger} c_{j\sigma}^p + h.c. - t'_p \sum_{\langle ij \rangle', \sigma} c_{i\sigma}^{p\dagger} c_{j\sigma}^p + h.c. \\ & + J \sum_{\langle ij \rangle} (\mathbf{S}_i^p \cdot \mathbf{S}_j^p - \frac{1}{4} n_i^p n_j^p), \end{aligned} \quad (2)$$

H_c describes the y -direction CuO chain:

$$H_c = -t_c \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{c\dagger} c_{j\sigma}^c + h.c. + J_c \sum_{\langle ij \rangle} (\mathbf{S}_i^c \cdot \mathbf{S}_j^c - \frac{1}{4} n_i^c n_j^c), \quad (3)$$

and H_I is the coupling between the plane and chain:

$$H_I = -t_\perp \sum_{ij\sigma} (c_{i\sigma}^{p\dagger} c_{j\sigma}^c + h.c.). \quad (4)$$

Here $\langle ij \rangle$ denotes the nearest-neighbor (NN) bond and $\langle ij \rangle'$ the next NN bond.

First, we use the slave-boson mean-field theory to decouple the Hamiltonians (2) and (3). Then, the coupling of the planar fermions to spin fluctuations are included via the random phase approximation (RPA). In the slave-boson approach, the creation operators of the planar and chain electrons $c_{i\sigma}^{p(c)\dagger}$ are expressed by slave bosons $b_i^{p(c)}$ carrying the charge and fermions $f_{i\sigma}^{p(c)}$ representing the spin, $c_{i\sigma}^{p(c)\dagger} = f_{i\sigma}^{p(c)\dagger} b_i^{p(c)}$. The mean-field order parameters are defined as $\Delta_{ij}^p = \langle f_{i\uparrow}^p f_{j\downarrow}^p - f_{i\downarrow}^p f_{j\uparrow}^p \rangle = \pm \Delta_p$, (\pm depend on if the bond $\langle ij \rangle$ is in the \hat{x} or the \hat{y} direction), $\chi_{ij}^{p(c)} = \langle f_{i\sigma}^{p(c)\dagger} f_{j\sigma}^{p(c)} \rangle = \chi_{p(c)}$. Notice that we do not assume any superconducting pairing in the chain at the mean-field level. The AF order in the chain is defined as $m_c = (-1)^i \langle S_{iz}^c \rangle$. At low temperatures we are concerned with, the boson condensation is assumed $b_i^{p(c)} \rightarrow \langle b_i^{p(c)} \rangle = \sqrt{\delta_{p(c)}}$, where $\delta_{p(c)}$ is the hole density in the plane (chain).

After Fourier transformation, the mean-field Hamiltonian of the planar and chain fermions can be written as

$$\begin{aligned} H_p = & \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}^p f_{\mathbf{k}\sigma}^{p\dagger} f_{\mathbf{k}\sigma}^p - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^p (f_{\mathbf{k}\uparrow}^{p\dagger} f_{-\mathbf{k}\downarrow}^{p\dagger} + h.c.) \\ & + 2N_p J_p (\chi_p^2 + \Delta_p^2), \end{aligned} \quad (5)$$

$$\begin{aligned} H_c = & \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}}^c f_{\mathbf{k}\sigma}^{c\dagger} f_{\mathbf{k}\sigma}^c + \varepsilon_{\mathbf{k}+\mathbf{Q}_c}^c f_{\mathbf{k}+\mathbf{Q}_c\sigma}^{c\dagger} f_{\mathbf{k}+\mathbf{Q}_c\sigma}^c) - 2J_c m_c \\ & \sum_{\mathbf{k}\sigma} \sigma (f_{\mathbf{k}\sigma}^{c\dagger} f_{\mathbf{k}+\mathbf{Q}_c\sigma}^c + h.c.) + 2N_c J_c (\chi_c^2 + m_c^2), \end{aligned} \quad (6)$$

where the summation over \mathbf{k} in the chain Hamiltonian is in the magnetic Brillouin zone (MBZ) due to the AF order, i.e., $-\pi/2 < k_y \leq \pi/2$. \mathbf{Q}_c is the one-dimensional

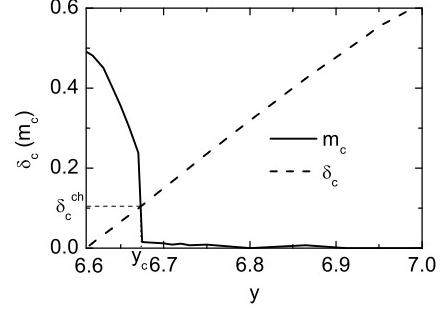


FIG. 1: The hole density δ_c (dashed line) and AF order m_c (solid line) in the chain versus the oxygen content y in YBa₂Cu₃O_y.

AF wave vector with $\mathbf{Q}_c = \pi/2$. $\varepsilon_{\mathbf{k}}^{p(c)}$ are given by $\varepsilon_{\mathbf{k}}^p = -2(\delta_t t_p + J'_p \chi_p)(\cos k_x + \cos k_y) - 4\delta_p t'_p \cos k_x \cos k_y - \mu_p$ and $\varepsilon_{\mathbf{k}}^c = -2(\delta_t t_c + J_c \chi_c) \cos k_y - \mu_c$, respectively. Correspondingly, the coupling of the planar and chain fermions can be written as

$$H_I = \tilde{t}_\perp \sum_{\mathbf{k}\sigma} (f_{\mathbf{k}\sigma}^{p\dagger} f_{\mathbf{k}\sigma}^c + h.c.). \quad (7)$$

The renormalized Green's functions for the planar fermions \hat{G}_p due to the coupling to spin fluctuations are calculated by Dyson's equation in the Nambu representation:

$$\hat{G}_p(\mathbf{k}, i\omega)^{-1} = \hat{G}_{p0}(\mathbf{k}, i\omega)^{-1} - \hat{\Sigma}_p(\mathbf{k}, i\omega), \quad (8)$$

where the self-energy can be obtained from [14],

$$\begin{aligned} \hat{\Sigma}_p(\mathbf{k}, i\omega) = & \frac{1}{\beta N_p} \sum_q \sum_{i\omega_m} J^2(\mathbf{q}) \chi_p(\mathbf{q}, i\omega_m) \hat{\sigma}_3 \\ & \hat{G}_{p0}(\mathbf{k} - \mathbf{q}, i\omega - i\omega_m) \hat{\sigma}_3, \end{aligned} \quad (9)$$

\hat{G}_{p0} is the bare Green's function obtained from the mean-field Hamiltonian and $\chi_p(\mathbf{q}, i\omega_m - \omega_m + i\delta)$ is the RPA-type spin susceptibility [14]. The Green's function for the chain fermions \hat{G}_c in the Nambu representation is obtained directly from the above mean-field Hamiltonian.

The real part of the optical conductivity $\sigma_1(\omega)$ is given by $\sigma_{1\alpha\alpha}(\omega)_{p(c)} = -\text{Im}\Pi_{\alpha\alpha}(\omega)_{p(c)}/\omega$ ($\alpha = \hat{x}, \hat{y}$). Here the imaginary part of the current-current correction function $\text{Im}\Pi_{\alpha\alpha}(\omega)_{p(c)}$ is expressed as

$$\begin{aligned} \text{Im}\Pi_{\alpha\alpha}(\omega)_{p(c)} = & \sum_{\mathbf{k}} \frac{\pi e^2}{N_{p(c)}} \int d\omega' [v_{\alpha}(\mathbf{k})_{p(c)}]^2 [f(\omega + \omega') \\ & - f(\omega')] \text{Tr}[\hat{A}_{p(c)}(\mathbf{k}, \omega + \omega') \hat{A}_{p(c)}(\mathbf{k}, \omega')], \end{aligned}$$

where v_{α} is the α -component of the quasiparticle group velocity and $\hat{A}_{p(c)}(\mathbf{k}, \omega)$ is the spectral function $[\hat{A}_{p(c)}(\mathbf{k}, \omega) = -(1/\pi)\text{Im}\hat{G}_{p(c)}(\mathbf{k}, \omega)]$.

In order to investigate the doping dependence of the optical conductivity, we need to determine the planar and chain doping density $\delta_{p(c)}$ for a given oxygen content y

in $\text{YBa}_2\text{Cu}_3\text{O}_y$. We determine δ_p versus y by using an empirical relation proposed recently by Liang *et al.* [16]. On the other hand, in the parent compound ($y = 6$), the valence of Cu ion in the CuO chain is +1, and thus the electron density in the chain is 2. Correspondingly, we may have a conservation condition $2 - n_c + 2\delta_p = 2(y - 6)$, which relates the chain electron density n_c and the planar doping density δ_p with y . From this condition, we can derive the chain doping density $\delta_c = 1 - n_c$ as a function of y , as shown in Fig.1. With the hole doping density, we can then solve the set of self-consistent equations for mean-field parameters $\chi_{p(c)}$, Δ_p , m_c , and $\mu_{p(c)}$. The input parameters are, $t_c = t_p = 2J$, $t'_p = -0.45t_p$, $J_c = J'_p = 3J/8$, $\tilde{t}_\perp = 0.1J$. The AF coupling constant J in the plane is used as the energy unit ($J \approx 130$ meV). The chain AF order m_c as a function of y at temperature $T \approx 0$ is shown as the solid line in Fig.1. We can see that the chain AF order m_c emerges with the decrease of the chain doping density and reaches its maxima value at $y = y_m = 6.61$ where the chain doping density is zero(half-filled) [17]. We note that the AF order has a step-like rise from a negligible value to about a half of its maxima at $y = y_c = 6.67$.

The chain optical conductivity for different oxygen content y is plotted in Fig.2. As y is increased to exceed $y_c = 6.67$ [Fig.2(a)], a prominent Drude-like peak at the dc limit shows up in the spectra, which indicates that the chain is superconducting. When the oxygen content y is decreased to $y = 6.67$, the Drude-like peak disappears and a finite frequency peak at $0.35J \approx 46$ meV occurs, leaving an excitation gap between this peak and the dc limit. This indicates that the system becomes insulating at this doping density. With further decrease of the oxygen content, the finite frequency peak will move to a higher energy, leading to a larger excitation gap. Meanwhile, the intensity of the spectra is suppressed heavily as shown in the inset of Fig.2(b). So, the superconductor-insulator transition occurs at $y = 6.67$, and the corresponding critical doping density in the chain is about $\delta_c^{ch} \approx 0.11$. This result is consistent quantitatively with the recent experimental data [11].

From Fig.1, one can see that the AF order is negligible or disappears (for $y > 6.9$) in the doping range where a Drude-like peak in the optical spectra is observed and has an appreciable value when the optical spectra show an insulating behavior. More importantly, at $y = y_c = 6.67$ where the insulator-superconductor transition occurs, the magnitude of AF order has a step like increase, i.e., it rises from a negligible value to nearly a half of its maximum. This shows clearly that the transition is associated with the emergence of the AF order. The occurrence of the AF order leads to a gap $2J_c m_c \approx 24.4$ meV in the single-particle energy band of the chain, i.e., a 48.8 meV excitation gap in the particle-hole excitations. This excitation gap suppresses the proximity effect coming from the coupling to the superconducting plane which is otherwise effective for $y > y_c$. Therefore, it is the competition between the AF order and the proximity effect

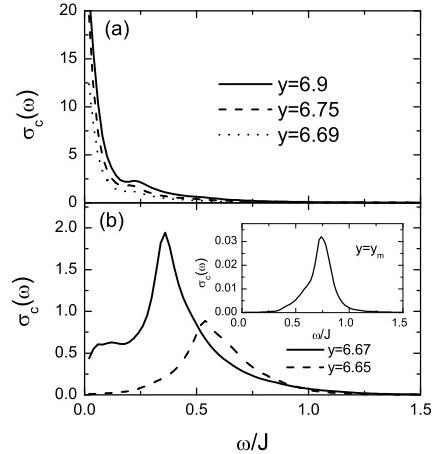


FIG. 2: The chain optical conductivity as a function of frequency in $\text{YBa}_2\text{Cu}_3\text{O}_y$ for different oxygen content y . The inset of Fig.(b) shows the spectra at $y = y_m = 6.61$ where the calculated chain doping density is zero(half-filled).

that leads to the superconductor-insulator transition in the chain.

When m_c equals to zero, the Hamiltonian for the system can be written as 4×4 matrix [14, 15]. The gap symmetry induced by the proximity effect may be examined by looking at the abnormal Green's functions of the chain electrons, $F_c(\mathbf{k}, \omega) = \sum_i U_{3i}(\mathbf{k}, \omega)U_{4i}(\mathbf{k}, \omega)/[i\omega - E_i(\mathbf{k}, \omega)]$, with $U_{4j}(\mathbf{k}, \omega) = \tilde{\Delta}_{\mathbf{k}}^p \tilde{t}_{\perp}^2 A_{j\mathbf{k}}/F_{j\mathbf{k}}$ and $\tilde{\Delta}_{\mathbf{k}}^p$ the superconducting gap in the plane with a $d_{x^2-y^2}$ symmetry [14]. Thus, the induced gap of the chain fermions is also of $d_{x^2-y^2}$ symmetry.

Now we study how the in-plane optical conductivity is influenced by the coupling to the chain. The real part of the in-plane optical conductivity $\sigma_1(\omega)$ is shown in Fig.3 for the superconducting [Fig.3(a-b)] and the normal state [Fig.3(c)], respectively. In the superconducting state, a Drude-like peak at the dc limit and a MIR hump around $\omega \sim J$ is evident from Fig.3(a) and (b), which reproduces what has been observed in the twinned samples [18]. These features are also consistent with previous theoretical calculations [19, 20, 21] in which only the in-plane electrodynamics is considered. A new feature observed here is that an extra peak emerges between the Drude-like peak and the MIR hump. Moreover, this extra peak disappears completely in the normal state, as seen from Fig.3(c). These results are consistent with the very recent experimental data [13]. We also note that there is only a weak $a - b$ anisotropy in the spectra around this peak. In the meantime, the in-plane spectra in the superconducting state are nearly isotropic both in the dc limit and in high frequencies. As a result, the plane-chain coupling does not cause an obvious in-plane anisotropy in the optical conductivity. Therefore, we expect that the anisotropy observed in experiments, which is obtained by subtracting the a -axis spectra from the b -axis spectra, is mainly contributed by the chain contribution.

Due to the coupling between the plane and chain, the

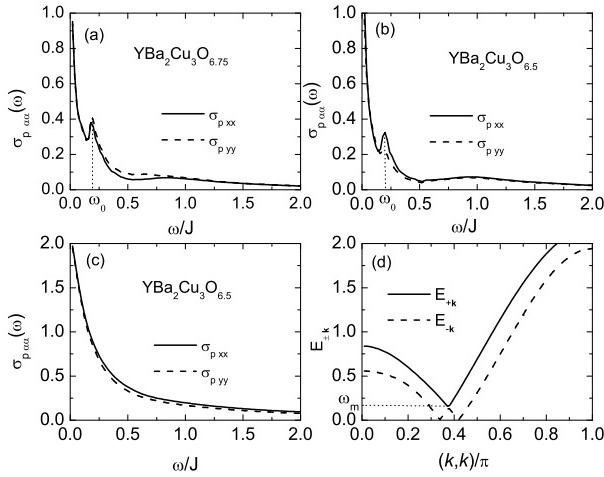


FIG. 3: Panels a)-c) plot the real parts of the in-plane optical conductivity as a function of frequency ω for different y . Panel a) shows the spectra for $y = 6.75$ sample in the superconducting state, panels b) and c) are the spectra for the ortho-II phase $y = 6.5$ sample with the planar doping density $\delta_p = 0.097$ [16] in the superconducting state at $T = 0.0005J$ and in the normal state at $T = T_c = 0.033J$, respectively. Panel d) shows the quasiparticle energy $E_{\pm k}$ along the diagonal direction in $YBa_2Cu_3O_{6.75}$.

energy band of quasiparticle is split into two branches with frequencies $E_{\pm k}$ [14]. In the superconducting state, the low-energy optical response comes mainly from the charge excitations around the nodal direction due to the presence of the superconducting gap. In Fig.3(d), we

plot $E_{\pm k}$ with k along the diagonal direction. Around the Fermi wave vector, there is a minimum $\omega_m \approx 0.18J$ in E_{+k} , and the band E_{-k} is below this minimum. When the excitation frequency is below ω_m , the optical response comes only from the E_{-k} . When $\omega \geq \omega_m$, an additional scattering channel from the band E_{+k} contributes to the response and leads to a peak around ω_m . In the normal state, the excitations near the entire Fermi surface are available, so that the minimum in E_+ varies at different wave vectors. As a result, the combined effect of these excitations causes no extra peak.

To summarize, we have elaborated that the competition of the plane-chain coupling and the antiferromagnetic order in the chain leads to the superconductor-insulator transition in the optical conductivity of the CuO chain. Specifically, the proximity superconductivity in the chain is induced by the plane-chain coupling while the insulating property is caused by the antiferromagnetic order. Meanwhile, we find an extra peak in the in-plane optical spectra at low frequencies in the superconducting state, which is between the Drude-like peak and mid-infrared component. This peak disappears in the normal state. These results are well consistent with the recent optical conductivity measurements.

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